Diethyl ether 60-29-7 | DTXSID3021720

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Mode	Data

Weighted KNN model

5-fold CV	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 4.72

Global applicability domain: Inside

Local applicability domain index: 6.17e-01

Confidence level: 6.89e-01

Nearest Neighbors from the Training Set

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Diethyl ether Measured: 5.37 Predicted: 4.72 Image not found

Methyl tert-butyl ether Measured: 1.51 Predicted: 3.67 Image not found

Triethylamine Measured: 4.90 Predicted: 5.95

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2-Nitropropane Measured: 8.32 Predicted: 7.41 Image not found

tert-Butyl alcohol Measured: 5.01 Predicted: 4.48